Methodology to address radioprotection and safety issues in the IFMIF/EVEDA accelerator prototype

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Abstract

In the IFMIF/EVEDA accelerator prototype, deuterons (with energies up to 9 MeV) interact with the materials of the accelerator components due to beam losses and in the beam dump, where the beam is stopped. The productions of neutrons/photons together with radioactive inventories due to deuteron-induced reactions are some major issues for radioprotection and safety assessment.

Here, we will focus on the proposal of a computational approach able to simulate deuteron transport and evaluate deuteron interactions and production of secondary particles with acceptable precision. Current Monte Carlo codes, such as MCNPX or PHITS, when applied for deuteron transport calculation, use built-in semi-analytical models to describe deuteron interactions. These models are found unreliable in predicting neutron and photon generated by low energy deuterons, typically present in the IFMIF/EVEDA prototype accelerator. In this context, a new computational methodological approach is proposed based on the use of an extended version of current MC codes capable to use evaluated deuteron libraries for neutron (and gamma) production.

The TALYS nuclear reaction code is found to be an interesting potential candidate to produce the evaluated data for double-differential neutron and photon emission cross sections for incident deuterons in the energy range of interest for IFMIF/EVEDA applications. The recently-released deuteron Talys-based Evaluated Nuclear Data Library, TENDL-2009, is considered a good starting point in the road to achieve deuteron data files of enough quality for deuteron transport problems in EVEDA.

Unfortunately, current Monte Carlo transport codes are not able to handle light ion libraries except for protons. To overcome this drawback the MCNPX code has been extended to handle deuteron (also triton, helion and alpha) nuclear data libraries. In this new extended MCNPX version called MCUNED, a new variance reduction technique has also been implemented for the production of secondary particles induced by light ions nuclear reactions, which allow reducing drastically the computing time needed in transport and nuclear response function calculations. Verification of these new capabilities for Monte

Carlo simulation of deuteron transport and secondary products generation included in MCUNED is successfully achieved.

The existence of the MCUNED code allows us for the first time testing the deuteron cross-section TENDL package by simulation of integral experiments. Some preliminary efforts are addressed to compare existing experimental data on thick target neutron yields for Copper with those computed by the MCUNED code using TENDL cross sections.

Introduction: IFMIF-EVEDA and radioprotection issues

The International fusion materials irradiation facility (IFMIF) [1] is one of the three projects of the fusion broader approach between Japan and the European Union, planned to be performed in parallel of ITER project. The objective of IFMIF is to study the behaviour under irradiation of materials and components in conditions close to a nuclear fusion reactor. Engineering validation and engineering design activities (EVEDA) [2] is the first phase of the IFMIF project and has begun in mid 2007. Engineering activities include the three main parts of the future IFMIF facility: the accelerator, the target and the tests facilities. A prototype of the IFMIF accelerator is under construction in Japan on Rokkasho-Mura site. The accelerator sub-systems and components will be provided by the European team that is in charge of safety and radioprotection calculations for these equipments.

The IFMIF-EVEDA prototype will be a 9 MeV, 125 mA CW deuteron accelerator, identical to the low energy section of one of the IFMIF accelerators. IFMIF will use two deuteron beam-lines delivering each 125 mA @ 40 MeV. The prototype will be tested to verify the validity of the design before launching the IFMIF construction. It includes an ion source, a Radiofrequency Quadrupole (RFQ) cavity and the first module of a superconducting Linac based on half wave resonator (HWR) cavities. As no target is foreseen for the accelerated beam, a beam dump (BD) is required to stop it during commissioning and accelerator tests.

Deuterons in the accelerator prototype will interact with materials all along the beam line where deuterons are lost, and at the end of the beam line, in the beam dump where the whole beam is stopped. As a result of these deuteron interactions with the intercepting material and with the previous deuterons implanted in it, secondary neutrons and gammas as well as deuteron induced activated products will be generated.

The generation of neutrons will induce: i) high neutron and gamma prompt dose rates during accelerator operation, ii) activation of the accelerator components as well as all the other materials inside the accelerator vault, including activation of air and corrosion products in the coolant, and iii) decay gamma dose rates after the accelerator shutdown. The deuteron induced activation of the accelerating components and beam stop will result in decay gamma dose rates after the accelerator shutdown. The production of tritium by interaction of deuterons with the previous implanted deuterium is also an issue to be considered.

The main elements of the methodology to address the abovementioned radioprotection issues (presented in the second section) can be grouped in two general sets: i) computational tools and nuclear data for transport of particles and calculation of relevant response functions, and ii) computational tools and nuclear data for activation calculations.

Here we will be focused on the transport activities, and in particular we will present the work done and final conclusions achieved within IFMIF-EVEDA ASG (Accelerator System Group) regarding the computational methodology designed to carry out the simulation of deuteron transport and secondary products generation.

Firstly, we present the outcome from a benchmark [3] performed to assess the availability and quality of cross section data for neutron generation due to incident deuterons. Calculations of excitation functions for deuteron reactions producing neutrons are performed using the nuclear models included in MCNPX [4] and PHITS [5], as well as the dedicated nuclear reaction code TALYS [6] and corresponding deuteron Talys-based Evaluated Nuclear Data Library TENDL2009 [7]. The definition of the benchmark is provided in the second section and the discussion of the results in the third one. It is shown that some developments regarding computational tools and nuclear data are required in order to solve the problem arising from the fact that the built-in nuclear models included in current MC codes do not allow predicting with a reasonable accuracy the production of secondary particles and residuals from deuteron interactions in the energy range of interest of the EVEDA accelerator. The potential advantages of using deuteron transport cross section data files produced by the dedicated nuclear model code TALYS in transport calculations, instead of using those built-in model includes inn the MC codes, is discussed in the third section.

The use of such tabulated data introduces the flexibility to change easily nuclear data used in the transport code when they need to be improved. Unfortunately, current Monte Carlo transport codes, such as MCNPX, PHITS or FLUKA [8], are not able to handle light ion libraries except for protons. To overcome this drawback the MCNPX code has been extended to handle deuteron, triton, helion and alpha nuclear data libraries. In this new extended MCNPX version, called MCUNED [9], a new variance reduction technique has also been implemented for the production of secondary particles induced by light ions nuclear reactions, allowing a drastic reduction in the computing time for many applications. The main features of MCUNED will be presented in the fourth section, showing its power in addressing like-EVEDA problems. The MCUNED code has been accepted by the ASG of IFMIF-EVEDA as the current MC transport option to use in addressing the deuteron transport problems in EVEDA.

The deuteron cross sections generated by TALYS, and in particular the recently-released deuteron files of ENDL-2009, it is considered a good starting point in the road to achieve deuteron data files of enough quality for deuteron transport problems in EVEDA and furthermore in IFMIF accelerators. The existence of the MCUNED code allows us for the first time testing the deuteron cross-section TENDL package by simulation of integral experiments. In the fifth section we present some preliminary efforts [10] aimed to compare existing experimental data on thick target neutron yields for copper with those computed by the MCUNED code using TENDL cross sections. Finally in the sixth section, main conclusions of the work are presented.

General methodology for radioprotection calculations: Need for validated nuclear data and computational tools

The main elements of the methodology can be grouped in two general sets: i) computational tools and nuclear data for transport of particles and calculation of relevant response functions, and ii) computational tools and nuclear data for activation calculations.

Different alternatives have been used in activation calculations for EVEDA applications. In all of them, the procedure followed is to use deuteron and neutron fluxes computed previously with transport codes as input to a dedicated activation code which will use activation cross section and decay data libraries. The MCNPX is used to transport the emitted gamma rays and compute flux and residual gamma dose rates. Some alternatives [11, 12] are under discussion within IFMIF-EVEDA ASG regarding the activation codes and activation cross sections to be used in EVEDA applications and the final agreement will be reached soon.

As far transport activities, the main items are the transport of deuterons, production and transport of secondary neutrons and gammas and finally the assessment of deuteron, neutron and gamma fluxes and prompt doses. The use of Monte Carlo transport codes has been the option consider for IFMIF-

EVEDA applications. Different options have been proposed to address the problem of deuteron implantation profile [12-14] which is necessary to be known to compute the d-D neutron source and tritium production. These options are under discussion within IFMIF-EVEDA ASG and the final agreement will be reached soon. The agreement has been already reached regarding the methodology to address the simulation of deuteron transport and secondary products generation. The presentation of the work done within this activity is the goal of this paper.

The Monte Carlo codes MCNPX and PHITS, widely used in radioprotection accelerator studies, were initially considered as candidates for EVEDA applications. These codes use built-in analytical models to deal with deuteron nuclear interactions. In some of the first EVEDA radioprotection studies aimed to the beam dump design, the applicability of MCNPX to predict neutron production with sufficient accuracy in the particular situation of 9 MeV deuterons impinging on the copper beam stop was found questionable [15]. As a consequence, a more extensive effort was planned in order to define a reliable methodology to calculate and make use of the deuteron cross sections needed for EVEDA calculations. In this context, a benchmark [3] has then been proposed between both European home teams involved in safety and radioprotection calculations for IFMIF-EVEDA (UNED and CEA) in order to compare calculated cross sections, using different MC transport codes and dedicated nuclear reaction codes, with experimental data available for different elements relevant to IFMIF-EVEDA project.

These elements are: Cu, Ni, Fe, W, C, Cr and Nb. They are typical components of accelerator equipments (Cu for the beam dump, stainless steel for the vacuum chamber, Nb and W for other specific equipments such as superconducting Drift Tube Linac). The benchmark has been focused on EVEDA phase and the energy has been set in the range 0 to 20 MeV.

The benchmark has then been performed into three steps:

- In the first step, an inventory of the available experimental data in EXFOR [16] regarding the excitation functions of the deuteron reactions producing neutrons for these elements has been undertaken.

- In the second step, the different cross sections have been calculated with the different nuclear models included in MCNPX and PHITS.

- In the third step, the different cross sections have been calculated with the dedicated nuclear reaction code TALYS.

The comparison of the results will allow us to test the MC codes regarding their capability to predict neutron production for EVEDA conditions and to test the capability of TALYS to generate neutron (and gamma) production data files for deuteron induced reactions with enough accuracy. The results obtained are discussed in the following section.

Description of deuteron interactions in the transport process: Limitations of current MC codes and potential of the TALYS nuclear reaction code

Cross sections calculated with MCNPX-2.6 (using INCL4/ABLA and ISABEL/Dresner/RAL model options) and PHITS (QMD model) show that for the majority of the reactions there are a very strong disagreement in both energy dependence profile and values. For the other nuclear models included in MCMPX (such as CEM03 and LAQGSM) the situation is even much worst. Thus, it turned out that the present version of the nuclear models included in MCNPX and PHITS are not appropriate for dealing with deuteron-induced reactions in the energy range of EVEDA applications.

Figures 1, 2 and 3 are examples of reactions showing the bad behavior of MCNPX and PHITS nuclear models. A strong disagreement with experimental cross sections is observed not only in amplitude but also in shape.

As far MCNPX, it is seen that the INCL4/ABLA model is in general the one providing the best results for EVEDA applications. ISABEL/Dresner/RAL is the second one in performance, but it is totally unacceptable. All the models, except INCL4, are unable to compute neutrons for deuteron incident energies below around 6 MeV, since as can be seen in the figures, unphysical very low values are assigned to the cross sections below this energy. In the EVEDA accelerator, the production of neutrons by interactions by 5 MeV deuterons in Copper is in terms of radioprotection implications an important aspect that should not be neglected [13, 17].

The general behavior of the TALYS-1.0 cross sections obtained using the default-global set of parameters is also illustrated in figures 1, 2 and 3. It is seen than even if results obtained with TALYS-1.0 (with default-global parameters) are in most of the cases not much better in amplitude than those obtained with MCNPX and PHITS, they give a shape that fits rather well the shape of experimental values. The utilization of TALYS with appropriate adjusting parameters will be required to obtain a good reproduction of experimental cross sections for safety and radioprotection calculations.

Several reactions, such as those given in figures 1, 2 and 3 (^{61}Ni(d,n)^{62}Cu, ^{65}Cu(d,2n)^{65}Zn and ^{64}Ni(d,2n)^{64}Cu, respectively) have been identified as examples of reactions for which a qualitative acceptable profile of the excitation function is obtained with TALYS-1.0 default-global parameters, but for which improvement in the fit to measurements is required.

Figure 1: Cross section for 61Ni(d,n)62Cu reaction: comparison of evaluated and measured data

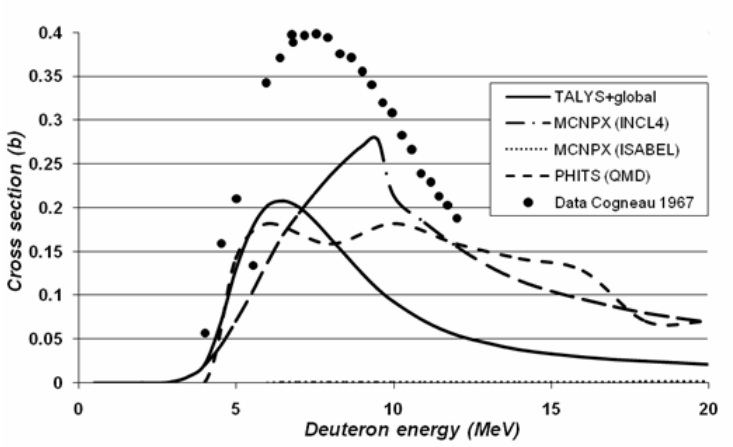


Figure 2. Cross section for 65Cu(d,2n)65Zn reaction: comparison of evaluated and measured data

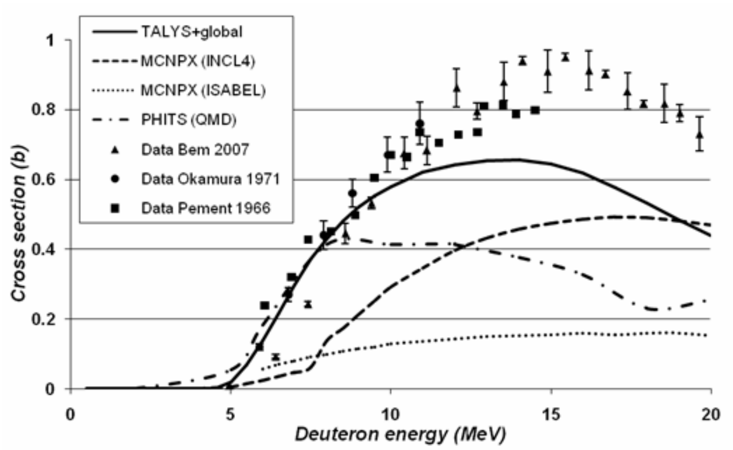
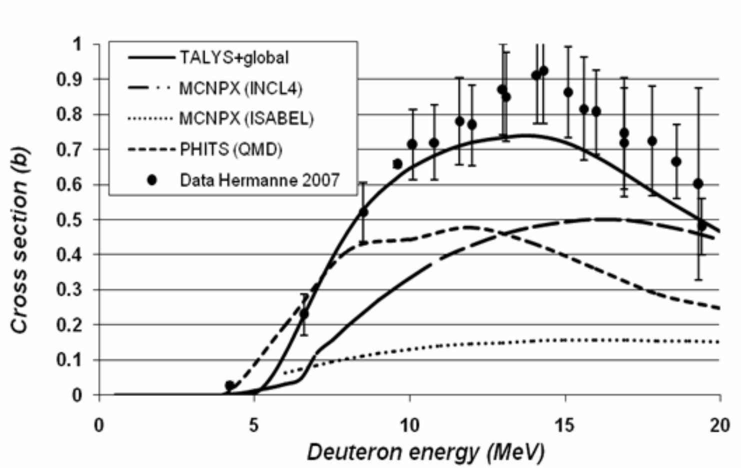


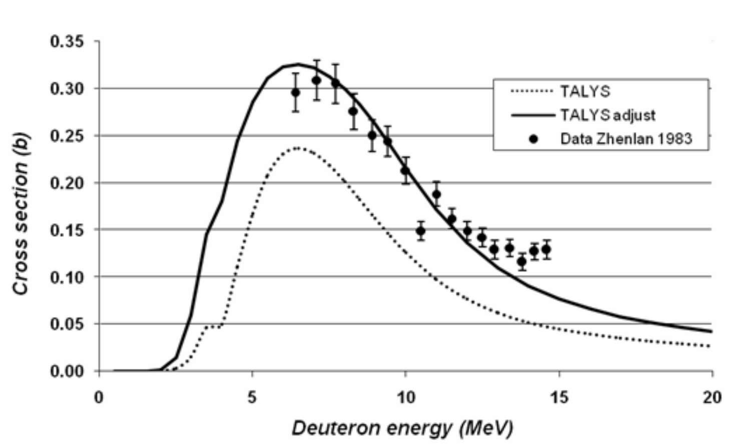
Figure 3. Cross section for 64Ni(d,2n)64Cu reaction: comparison of evaluated and measured data



For these problematic cases, TALYS offers the capability to adjust the parameters of the optical model potential (OMP) involved in the interactions between the incident particle and the nucleus. In order to show that these kinds of problems can be solved reasonably, we have chosen two cases. In the first one, results of fitting using standard mathematical tools is presented. In the second one, results obtained from using local parameters based in a sound physical approach are given.

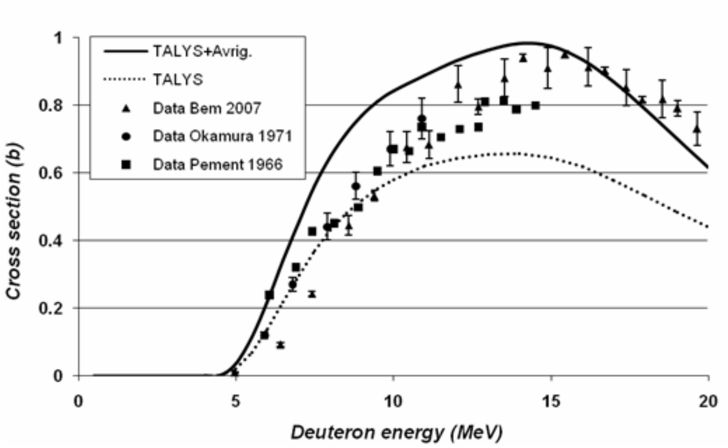
The first case addresses deuteron reactions in ^{56}Fe. For this nuclide there are values in EXFOR for three different reactions: ^{56}Fe(d,n)^{57}Co, ^{56}Fe (d,2n)^{56}Co, and ^{56}Fe (d,a)^{54}Mn. The TALYS-1.0 results (using default-global parameters) obtained for them show that they reproduce well the energy dependence of the cross section defined by experimental data but that the quantitative fit is not good enough. Fitting calculations with standard mathematical tools were done by the UNED team for all the experimental values [3] and as a result a common set of parameters for the three reactions have been derived. Figure 4 shows the improvement performed for the reaction ^{56}Fe(d,n)^{57}Co using TALYS-1.0 with the fitting parameter set over the TALYS-1.0 results using the default-global parameters. With the selected parameter set, an improvement of ^{56}Fe (d,2n)^{56}Co and ^{56}Fe (d,a)^{54}Mn reactions –of interest for activation analysis- has also been achieved.

Figure 4. Improved cross section for reaction 56Fe(d,n)57Co with TALYS & fitting OMP parameters



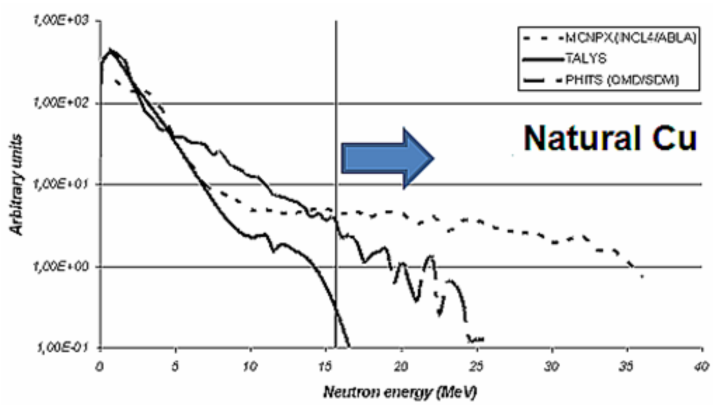
The second case refers to the $^{65}Cu(d,2n)^{65}Zn$ reaction for which Avrigeanu local OMP parameters derived from physical basis are used [18]. The improvement of the fitting is also observed (see figure 5).

Figure 5. Improved cross section for reaction 65Cu(d,2n)65Zn with TALYS & local OMP parameters



Other critical issue in regards to neutron production is the emitted spectrum. It is worthy mention that the one computed with MCNPX-2.6 and PHITS is not realistic at all because an unphysical high energy tail is predicted, on the contrary, TALYS-1.0 predictions are always consistent with the kinematics of the reactions. An example of this is provided in figure 6, that shows the angular integrated distribution for 9 MeV deuterons incident on natural Copper computed by MCNPX-2.6 (INCL4/ABLA), PHITS and TALYS-1.0 (default-global parameters) The maximum physical energy of the emitted neutrons is about 15.7 MeV.

Figure 6: Probability distribution of emitted neutrons for Cu^{nat} and 9 MeV incident deuterons



As a conclusion of this benchmark exercise, it was agreed within the ASG of IFMIF-EVEDA that the option to follow for addressing transport simulations and prompt dose calculations in EVEDA was the development of a computational procedure based on extending Monte Carlo codes to use external data files generated by TALYS, with appropriate adjusting optical model potential parameters when necessary.

MCUNED: New capabilities for Monte Carlo simulation of deuteron transport and secondary products generation

MCUNED [9] is a new computational tool resulting from an extension of the MCNPX code, which improves significantly the treatment of problems where any secondary product (neutrons, photons, tritons, etc.) generated by low-energy deuteron induced nuclear reactions could play a major role. The two singular features of MCUNED are: i) it handles deuteron evaluated data libraries (residual production cross-sections and energy-angle distributions of all outgoing particles) and ii) it includes a reduction variance technique for production of secondary particles by charged particle-induced nuclear interactions, which allow reducing drastically the computing time needed in transport and nuclear response calculations. A third feature is that MCUNED input is fully compatible with any MCNPX input and all the capabilities of the original MCNPX (like the flexibility in definition of the charged particle source, the definition of the geometry of the system, ptrac option, nuclear responses, etc) are available in the MCUNED version. Moreover the responses of MCUNED simulations have not experienced any variation with the implementation of the new capabilities respect to MCNPX responses. In the following we present some aspects of the two singular features of MCUNED.

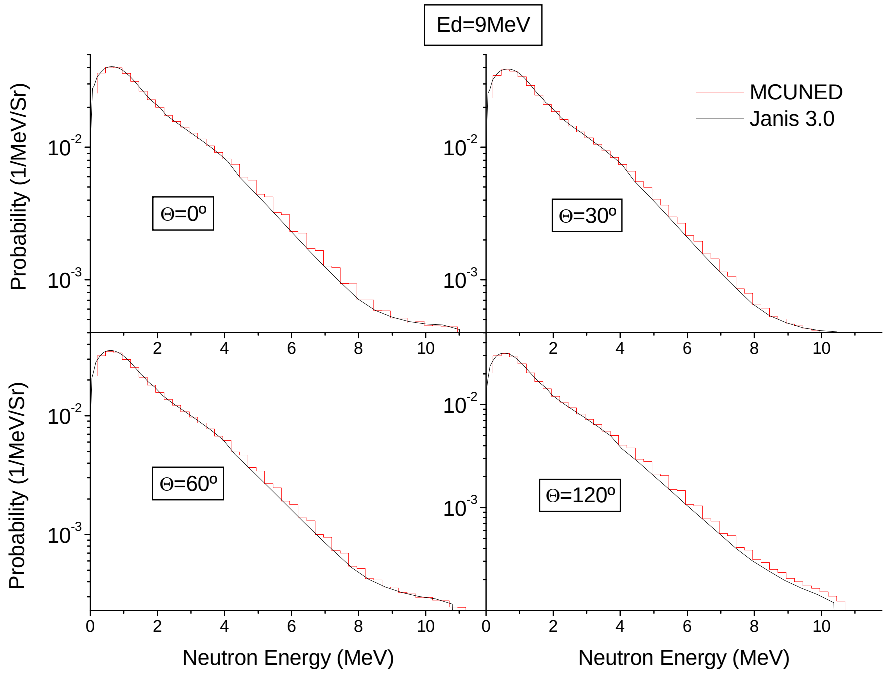
Handling of deuteron libraries for transport calculation: implementation in MCPNX and verification process

The MCNPX subroutines devoted to read and process proton nuclear cross-section from libraries have been modified and extended allowing the use of deuteron libraries. Subroutines dedicated to the sample of nuclear reactions have been also modified in order to use tables instead of models during the deuteron transport. The charged particle transport scheme remains the original from MCNPX.

A verification process has been defined in order to check that the modification of MCNPX subroutines allowing reading deuteron libraries is correct. The verification test is defined by a setup consisting of 9 MeV deuteron pencil beam impacting onto a thin cylindrical Cu-63 target. Simulations are performed to obtain the neutron spectra emitted from the thin target at different angles respect to the beam axis. The simulations are performed with MCUNED and the deuteron transport library is provided by the TENDL package [7]. Double differential neutron yields computed by MCUNED are straightforward converted to double differential cross-sections and compared with the double differential cross-section supplied by TENDL. The matching between both results was excellent. This outcome validates the management of deuteron cross-section tables in MCUNED.

Figure 7 shows the neutron emission double differential cross-section obtained from ENDF format library and the cross-section calculated with MCUNED for four different angles, showing the excellent matching between both.

Figure 7: Neutron double differential cross section for the reaction d-Cu63 and 9 MeV deuterons.



Variance reduction technique for generation of secondary product by light ions interaction: basis and verification

Another important drawback of current Monte Carlo codes when applied to transport of low-energy light ions is the huge amount of computing time that can be required to address some important problems. This will take place in problems where one or several types of secondary products play a major role. A good example is the calculation of prompt dose rates outside the accelerator vault and corresponding shielding issues. The neutrons produced by deuteron interactions are the main responsible for these doses.

In this kind of problems the interest of the simulation is emphasized in the transport of secondary particles, and it is necessary to perform the calculation with a large number of secondary particles histories in order to reduce the statistical error in the response functions of interest (doses in shielding problems). Moreover, the secondary particles source has to be distributed adequately (energetically and spatially) with respect to the simulated primary particle source. Let name by SH the desired number of secondary particles histories to achieve an acceptable statistical error. If we represent the production of secondary per primary particles by (s/p), then the number of needed primary particles histories PH can be written as $SH^*(s/p)^{-1}$.

The problem arises when the production of secondary per primary particles (s/p) is very low. For example, if primary particles are low energy ions, such as deuterons in the EVEDA (maximum energy is 9 MeV) where the number of produced neutrons per incident deuteron is about 10^{-4}, the problem highlighted above takes a real importance. This problematic of scarce secondary particle production has been successfully treated in [19] for a specific geometry and beam-target setup, but clearly the method is too restricted to be used in a general case.

At low energy, ions have short track lengths inside the material due to the slowing down of the particle. This short track associated with a relatively low absorption cross section leads to a very low production of secondary particles. In EVEDA the order of magnitude of the ratio (s/p) will be around 10^{-4}. This feature of low-energy light ion transport means to waste a lot of computing time in transporting primary particles that have no contribution in the calculation of the response functions associated to the production and transport of secondary particles.

The main idea of the new variance reduction technique [9] implemented in MCUNED, for the production of secondary particles from nuclear reaction with charged particles, is to always force the nuclear reaction, taking care of the correct transport of charged particle, giving rise to the absorption of the incident particle by the target nucleus for each charged particle history. The weight of the secondary particle produced is then multiplied by the probability of such nuclear absorption, in order to keep the yield of secondary particle production. This variance reduction technique is valid for all kind of ions, but it is not suitable for electron or positron because it does not take into account bremsstrahlung effect which is negligible for ions.

A comprehensive verification process has been undertaken [9] and the procedure to evaluate the benchmark test set for verification of the variance reduction technique is based in the following considerations:

i) Simulations are run with MCNPX and MCUNED. The same inputs files are used in both simulations. The only differences will be the card in the MCUNED input setting active the option of variance reduction for generation of secondary particles, and the different number of primary particles histories used in running MCNPX and MCUNED.

ii) The number of initial primary particles histories in both simulations is adjusted to achieve the same (or very similar) statistical error in the tally results of interest.

iii) The Variance reduction technique is considered correct if the relative error between MCNPX and MCUNED calculations is comparable to the statistical error of the tally values, that is:

$$\varepsilon_r = \frac{\left| \overline{X}_{MCNPX} - \overline{X}_{MCUNED} \right|}{\overline{X}_{MCNPX}} \leq max\left(\varepsilon_{MCNPX}, \varepsilon_{MCUNED}\right)$$

where $\overline{X}_{MCNPX}$ is the mean value of a given quantity computed by MCNPX, $\overline{X}_{MCUNED}$ is the mean value of the same quantity computed with MCUNED having active the option of variance reduction technique, and ε_{MCNPX} and ε_{MCUNED} are the statistical errors in MCNPX and MUNED calculations.

iv) Finally, in order to measure the benefit in using the variance reduction technique, we will compare the computing time necessary to perform the whole simulation with one processor computer when running MCNPX and MCUNED.

The conclusion of the verification process performed is that variance reduction technique leads to correct results and that is useful when the production of secondary particle is low and essential when the production rate of secondary particle is very low.

As an example of the kind of tests performed, we will refer to that in which a 10MeV proton beam impacts onto a cylindrical copper target, 1mm thickness and 1 cm radius. Simulations are performed with MCNPX and MCUNED to obtain neutron spectrum at different angles respect to the beam axis, using in both simulations an external data library for protons reaction cross sections.

The comparison between MCNPX and MCUNED calculations for the emitted neutrons from the thick target relative to spectral neutron yield, energy integrated angular distribution of neutron yield and neutron energy spectra at different emission angles shown that the relative errors between MCNPX and MCUNED mean values are lower than the statistical errors (statistical errors lower than 1% in most of the values). The good agreement between both simulations traduces the correct implementation of the variance reduction technique into the MCUNED code.

In Table 1 the number of histories used and results from both simulations are displayed to exhibit the benefit in using the variance reduction technique. It is seen that the reduction in computing time is in this case outstanding, being the time needed by MCNPX three orders of magnitude higher than with MCUNED simulation.

Table 1: MCNPX-MCUNED performance comparison of neutron emitted from Copper thick target. The computing time is the time necessary to perform the whole simulation with one processor computer**.**

	MCNPX	**MCUNED**
Number of histories	1E+10	1E+10
Computing time	1.37E+05 minutes	32 minutes
Produced neutron histories	5.59E+06	5.36E+06
Neutron/proton	5.589E-04	5.587E-04
Statistical error	0.04%	0.03%

An estimation of the ratio between the computing time used without (normal execution of MCNPX) and with variance reduction can be made straightforward. Taking T_p as the computing time it takes to calculate one primary particle history and T_s the time it takes to transport the secondary particles produced by the source particle nuclear reaction, then the time needed to produce and transport secondary particles without variance reduction will be $T_{withoutVR}= n*T_p + T_s$ (with $n=(s/p)^{-1}$), while with variance reduction the new time is $T_{VR}=T_p+T_s$. The time saving gain is then $G = \frac{T_{withoutVR}}{T_{VR}} = \frac{n + T_s / T_p}{1 + T_s / T_p}$.

Since, for the low energy deuterons present in EVEDA, the number of secondary neutrons per incident deuteron is in the order of 10^{-4} for 9 MeV deuterons, a very important gain higher than a factor 1000 will be obtained for most of the applications.

Other tests have been performed [9] to check the ability of the variance reduction technique to reproduce in addition to the secondary neutron the photon production, neutron and photon fluxes, as well as response functions related to these quantities, such as the ambient equivalent dose produced by neutrons and photons in the surroundings of a thick target. The simulation setup consists of a 100 mA proton current at 6.7 MeV impinging on a cylindrical nickel target of 1mm thickness and 1cm radius. This simulation has the characteristics parameters of the beam stop irradiation conditions of the LEDA accelerator. The results of the simulations have shown the positive verification of the implementation of the reduction variance technique for calculation of all kind of response functions.

TENDL deuteron library benchmarking against integral experimental data: Applications to Copper

We present the outcome of preliminary efforts [10] aimed to compare existing experimental data on thick target neutron yields for deuteron interactions on copper with those computed by the MCUNED code using TENDL-2009 deuteron cross sections [7]. Experiments for incident deuterons energy up to 40 MeV have been collected.

The experimental and simulated results for the neutron yields are summarised in tables 2 and 3.

Table 2: Total neutron yield (4π)

Ref	E_d (MeV)	E_n> (MeV)	Exp (n/d)	TENDL (n/d)	Yield Frac.
20	10	0	8.81E-04	6.44E-04	1
21	33	0	1.81E-04	1.50E-02	1

Table 3: Neutron yield in the forward direction

Ref	E_d (MeV)	E_n> (MeV)	Exp (n/d)	TENDL (n/d)	Yield Frac.
22	16	4	2.76E-04	5.94E-05	0.20
21	33	4	6.16E-03	7.49E-04	0.39
22	33	4	6.68E-03	7.49E-04	0.39

The measured total yield including all neutron energies is in reasonable agreement with the simulations. The major component of the discrepancy between experiments and simulations has to do with the neutron yield in the forward direction. Then, it can be said that TENDL underestimates neutrons emitted in the forward direction.

The neutron spectrum in the forward direction for two different energies is depicted in figure 8. It can be seen that is not correctly reproduced by TENDL, increasing the discrepancies as deuteron energy increases.

Figure 8: Spectra of neutrons emitted in the forward direction (experiments from ref. 22)

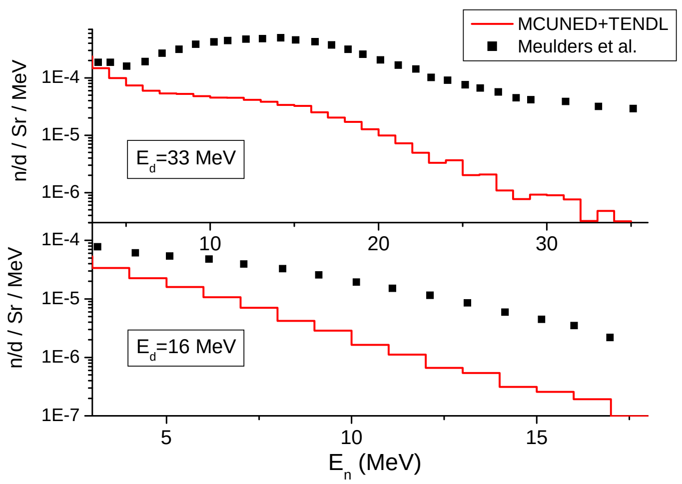
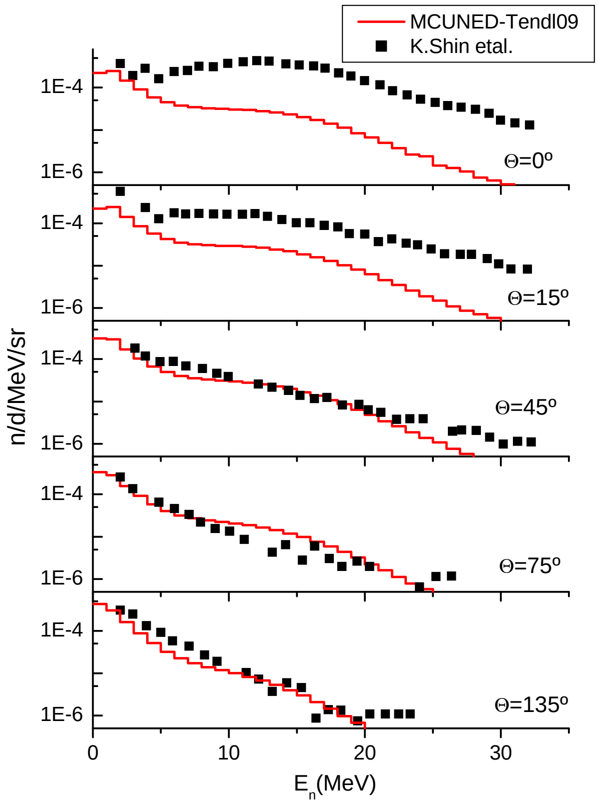


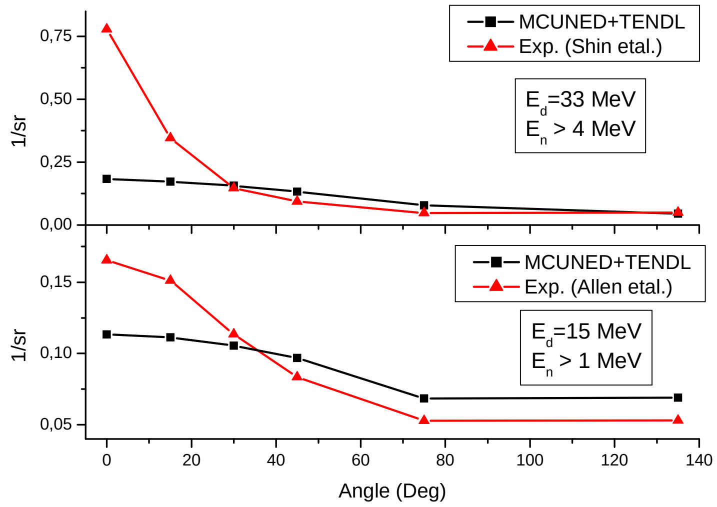
Figure 9 shows the neutron spectra at various emission angles for 33 MeV incident deuterons. This figure shows that up to 45 degrees the simulated and experimental spectra do not match each other. For backward neutrons, from 45 degrees and higher, the simulated and experimental spectra are in good agreement.

Figure 9: Neutron spectra produced by 33 MeV deuterons (experiments from ref. 21)



The angular distribution of produced neutron has been plotted in figure 10 for two different energies. For both incident deuteron energies, the experimental and simulated angular distributions are similar for angles higher than 45 degrees, while in forward direction the experimental distribution has a stronger contribution, being the discrepancies much lower as deuteron energies decreases.

Figure 10. Normalized neutron angular distribution (experiments from ref. 21, 23)



The differences existing between experimental and simulated spectra can be attributed to the deuteron break-up process during the nuclear reaction. The hump at 13 MeV in figure 9 at 0 degrees is the typical signature of the break-up process, which can be defined as having a projectile fragment emerging from the reaction in a relatively narrow peak centred close to the beam velocity and strongly directed toward forward angles. Since break-up process is included in TALYS with a simple model, then the TENDL deuteron library should reproduce this behaviour. Angular integrated neutron spectra produced by TALYS exhibit the break-up hump feature, but the code is not able to reproduce correctly the angular spectra. In fact, to produce the angular neutron spectrum, TALYS use the Kalbach [24] systematic. It is known that this systematic cannot reproduce satisfactorily the peaked forward angular distribution and instead of producing a pronounced break-up contribution to the forward angle, this systematic smoothes the break-up contribution over a large angular aperture. Very recently a new phenomenological model for projectile break-up reaction has been proposed [25]. In this model a peaked forward angular distribution is given to reproduce the angular distribution of the emitted fragment of the break-up reaction. Experiments recently performed [26] for copper in the energy range of interest for EVEDA will be extremely useful (since the few experiments available in this energy range) in evaluating and improving (if necessary) TENDL for EVEDA applications.

Conclusions

The different computational elements required in addressing the radioprotection issues of the IFMIF-EVEDA accelerator prototype have been identified and several alternatives have been found for most of them. Some of the possible options are under discussion within IFMIF-EVEDA ASG regarding activation and deuterium implantation issues and a final agreement will be reached soon.

Regarding simulation of deuteron transport and secondary products generation the agreement about the computational methodology to be used is already reached. It has been concluded the following: i) the nuclear reaction models included in the transport codes (MCNPX, PHITS) should not be used in EVEDA radioprotection calculations, ii) the cross-sections for deuteron reactions should be calculated with the dedicated nuclear model reaction code TALYS, using when necessary appropriate adjusting OMP parameters to achieve a better description of the nuclear reactions of interest for EVEDA, iii) extensions of current transport Monte Carlo codes are needed in order to include the capability to use the deuteron evaluated transport data files generated by TALYS, and iv) MCUNED code, a MCNPX extended version, is the accepted response to this need.

The two singular features of MCUNED are: i) it handles deuteron evaluated data libraries (residual production cross-sections and energy-angle distributions of all outgoing particles),and ii) it includes a reduction variance technique for production of secondary particles by charged particle-induced nuclear interactions, which allows reducing drastically the computing time needed in transport and nuclear response calculations. Around a factor of 1000 in saving computing time can be obtained with MCUNED for EVEDA applications. All the MCUNED extensions to MCNPX have been verified with very positive results.

MCUNED-TENDL libraries shows a relevant superior performance versus current Monte Carlo simulation tools for deuteron transport in the EVEDA energy range, but this performance may be needed to be improved by adjusting Deuteron-TENDL library cross sections when required.

MCUNED is the only tool available to perform benchmarking of the TENDL evaluated deuteron cross section against integral experiment.

Efforts are underway for benchmarking of TENDL-2009 against experimental data on thick target neutron yields for deuteron interactions on copper. Experimental values are compared with those obtained by simulation of the experiments using the MCUNED code and TENDL-2009 deuteron cross sections. Experiments for incident deuterons in the range of energies of interest for EVEDA and IFMIF accelerators have been collected. Total neutron yields from simulations are in a reasonable agreement with experiments, but TENDL underestimates neutrons yields emitted in the forward direction. Angular distribution and spectrum of backward-emitted neutron is well reproduced by TENDL but the neutron spectra is not well reproduced for neutrons emitted in the forward direction.

Differences between experiments and simulations decreases as incident deuteron energy decreases, and a reasonable behavior of TENDL library could be expected for EVEDA applications. Unfortunately few experiments exist for EVEDA applications. The simulation of those recently performed for 9 MeV deuterons on copper will be very useful in evaluating and improving (if necessary) TENDL for EVEDA applications.

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References

[1] "IFMIF Comprehensive Design Report", by the IFMIF International Team, an activity of the International Energy Agency, Implementing Agreement for a Program of Research and Development on Fusion Materials, January 2004.

[2] P. Garin, M. Sugimoto, "Main baseline of IFMIF/EVEDA project", *Fusion Engineering and Design*, **84**, 259 (2009).

[3] V. Blideanu, M. García, P. Joyer, D. López, A. Mayoral, F. Ogando, F. Ortíz, J. Sanz and P. Sauvan, "Deuteron cross section evaluation for safety and radioprotection calculations of IFMIF/EVEDA accelerator prototype". Proceedings 14th ICFRM, Sapporo, Japan, Sep. 6-11, 2009.

[4] D.B. Pelowitz, ed.: 'MCNPX: User's manual, v2.6.0', LA-CP-07-1473 (April 2008) http://mcnpx.lanl.gov

[5] Iwase, H. And Niita, K. 'PHITS: Particle and Heavy-Ion Transport code System. Version2.08'. (2006). http://phits.jaea.go.jp/

[6] A.J. Koning, S. Hilaire and M.C. Duijvestijn, "TALYS-1.0", Proc. of the Int. Conference on Nuclear Data for Science and Technology (ND2007), April 22-27 (2007) Nice, France, editors O.Bersillon, F.Gunsing, E.Bauge, R.Jacqmin, and S.Leray, EDP Sciences pp 211-214 (2008). & "Talys 1.2. User Manual" (2009). http://www.talys.eu/home/

[7] A.J. Koning, S. Hilaire, M.C. Duijvestijn, http://www.talys.eu/tendl-2009/

[8] A. Ferrari, P.R. Sala, A. Fasso and J. Ranft, 'FLUKA: a multi-particle transport code', CERN 2005-10 (2005), INFN/TC_05/11, SLAC-R-773, http://www.fluka.org/fluka.php

[9] P. Sauvan, J. Sanz, F. Ogando, "New capabilities for Monte Carlo simulation of deuteron transport and secondary products generation", *Nucl. Inst. and Meth. A*, **614**, 323 (2010).

[10] P. Sauvan, A. Mayoral, J. Sanz, A. J. Koning, F. Ogando, M. García, D. López, A. Ibarra, "Computational tools and nuclear data for radioprotection studies in low energy light ions accelerators". International conference on Nuclear Data for Science & Technology (ND2010), JeJu, Korea, April 2010.

[11] J. Sanz, O. Cabellos and N. García-Herranz, 'ACAB -2008: Activation Code V2008', Nuclear Energy Agency NEA Data Bank. NEA-1839, (2008).

[12] P. Joyer, J-M. Dumas, V. Blideanu, J. Sanz, M. García, A. Mayoral, "IFMIF / EVEDA accelerator nuclear safety issues and nuclear data needs", Proc. Shielding Aspects of Accelerators, Targets and Irradiation Facilities (SATIF-9) ORNL SNS, Oak Ridge, TN, USA. (2008).

[13] J. Sanz, M. García, P. Sauvan, D. López, C. Moreno, A. Ibarra, L. Sedano, "Neutron induced activation in the EVEDA Accelerator materials: Implications for the accelerator maintenance". Journal of Nuclear Materials 386–388 (2009) pp.991–993.

[14] A. Mayoral, J. Sanz, P. Sauvan, D. López, M. García, F. Ogando, "Relevance of d-D interactions on neutron and tritium productions in IFMIF-EVEDA prototype". 14th International Conference on Fusion Reactor Materials (ICFRM-14), Sapporo (Japan), September 6-11 (2009).

[15] J. Sanz, M. García, F. Ogando, A. Mayoral, D. López, P. Sauvan, B. Brañas, "First IFMIF/EVEDA radioprotection studies for the preliminary design of the accelerator beam dump". Fusion Science and Technology, Vol.56, N.1 (2009) 273-280.

[16] EXFOR Systems Manual, IAEA-NDS-207 (BNLNCS-63330-00/04-Rev.).

[17] M. García, J. Sanz, P. Sauvan, F. Ogando, D. López, C. Moreno, A. Mayoral, V. Blideanu, C. Moreno, “Decay Gamma Dose Rates in the EVEDA accelerator: Impact of the deuteron losses uncertainties in the accelerator maintenance”. Nuclear Technology / Volume 168 / Number 1 / October 2009 / pp. 132-138.

[18] M. Avrigeanu, V. Avrigeanu and Fl. Roman, “Deuteron-induced activation cross section evaluation for accelerator materials”. Progress Report to the EURATOM-MEdC Association. Task: TW5-TTMI-004, Deliverable No. 6 December (2006).

[19] M. García, F. Ogando, P. Ortego, J.M. Arroyo, B. Brañas, C. Töre, D. López, P. Sauvan, A. Mayoral, J. Sanz, "Optimized design of local shielding for the IFMIF/EVEDA beam dump", Proceedings of this conference.

[20] L.W. Smith and P.G. Kruger, “Thick Target Yields from (d,n) Reaction at 10 MeV”, *Physical Review*, **83**, 1137, (1951).

[21] K. Shin, et al., “Neutron and photon production from thick targets bombarded by 30-MeV p, 33-MeV d, 65-MeV ^{3}He and 65-MeV α ions: Experiment and comparison with cascade Monte Carlo calculations”, *Physical Review C*, **29**, 1307, (1984).

[22] J. P. Meulders, P. Leleux, P.C. Macq and P. Pirart, “Fast Neutron Yields and Spectra from Targets of Varying Atomic Number Bombarded with Deuterons from 16 to 50 MeV”, *Phys. Med. Biol.*, **2**, 235, (1975).

[23] A. J. Allen et al., “Thick Target Fast Neutrons Yield from 15-MeV Deuteron and 30-MeV Alpha-Bombardement”, *Physical Review*, **81**, 536, (1951).

[24] C. Kalbach, “Systematics of continuum angular distributions: Extensions to higher energies”, *Physical Review C*, **37**, 2350, (1988).

[25] C. Kalbach, “Complete Phenomenological Model for Projectile-Breakup Reactions”, http://www-nds.iaea.org/fendl3/docs/dBreakupRCM2.pdf (2010).

[26] Nobuhiro Shigyo, “Measurement of Deuteron Induced Thick Target Neutron Yields at 9 MeV” , International conference on Nuclear Data for Science & Technology, JeJu, Korea, April 2010.